Nanoscale Study of the Phase Decomposition in Model Ni-Al-Cr Superalloys

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Project Background

- Part of a larger study of model Nickel-base superalloys involving experimental and simulated results for [1-5]:
  - Ternary Ni-Al-Cr alloys
  - Quaternary Ni-Al-Cr-Re, Ni-Al-Cr-Ru, Ni-Al-Cr-W, and Ni-Al-Cr-Ta alloys

[1] Sudbrack CK. Ph.D. thesis, Northwestern University, Decomposition Behavior in Model Ni-Al-Cr-X Superalloys:Nanostructural Evolution and Compositional Pathways, December 2004.
[2] Yoon KE. Ph.D. thesis, Northwestern University, Temporal Evolution of the Chemistry and Nanostructure of Multicomponent Model Ni-Based Superalloys, June 2004.
[3] Booth-Morrison C, Weninger J, Sudbrack CK, Noebe RD, Seidman DN. Effect of solute Concentrations on the Kinetic Pathways in Ni-Al-Cr Alloys. to be submitted to Acta Mat. 2006.
[4] Mao Z, Sinnott SB, Martin G, D.N. S. Determination of Pair-Wise Interaction Energies and the Calculation of Ternary Phase Diagrams of Ni-Al-Cr Alloys by First-Principles Calculations. to be submitted to Acta Materialia 2006.
[5] Mao Z, Sudbrack C, Yoon K, Martin G, Seidman D. Diffusion Mechanism as a Selection Process for Nucleation, Growth and Coarsening Pathway in Multicomponent Concentrated Alloys. submitted to Nature Materials 2006.

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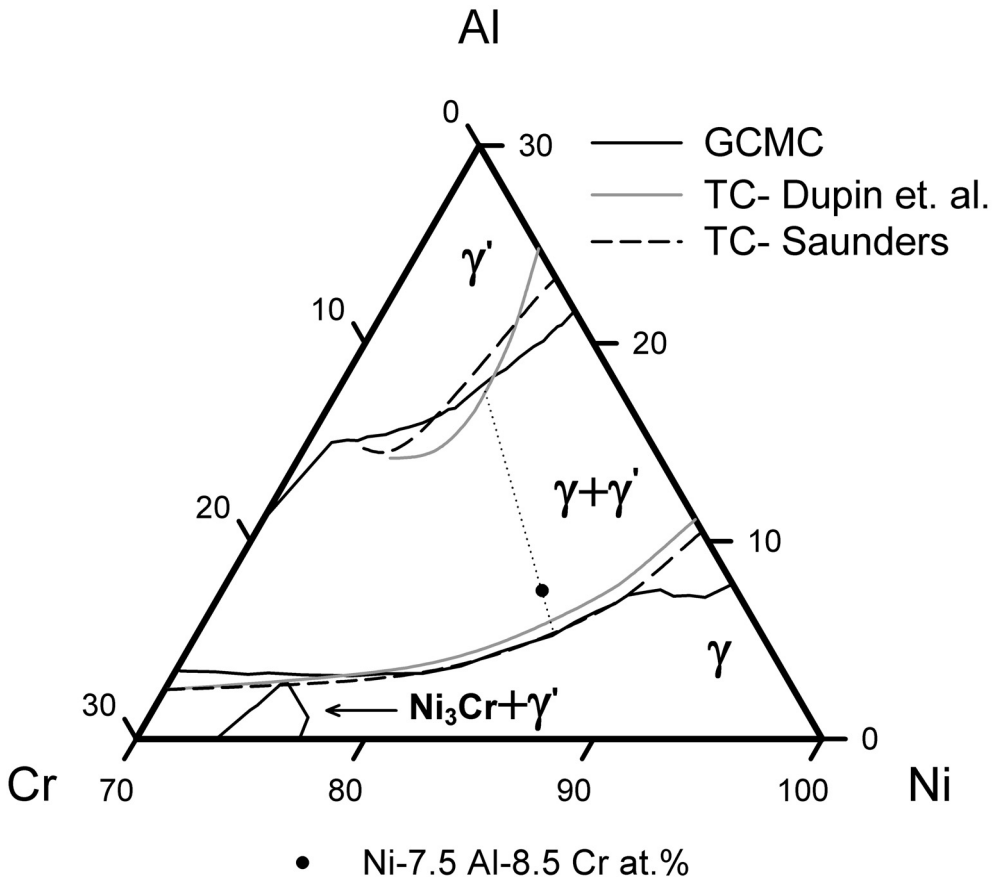
Ni-7.5 Al-8.5 Cr at.% @ 600°C

- Ni-7.5 Al-8.5 Cr at.% was designed to have relatively low equilibrium volume fraction of precipitates (φ^{eq}) of ca. 15% at 600°C
- This will allow us to study the nucleation, growth and coarsening of the γ'-precipitate phase by atom-probe tomography



[4] Mao Z, Sinnott SB, Martin G, D.N. S. Determination of Pair-Wise Interaction Energies and the Calculation of Ternary Phase Diagrams of Ni-Al-Cr Alloys by First-Principles Calculations. to be submitted to Acta Materialia 2006.

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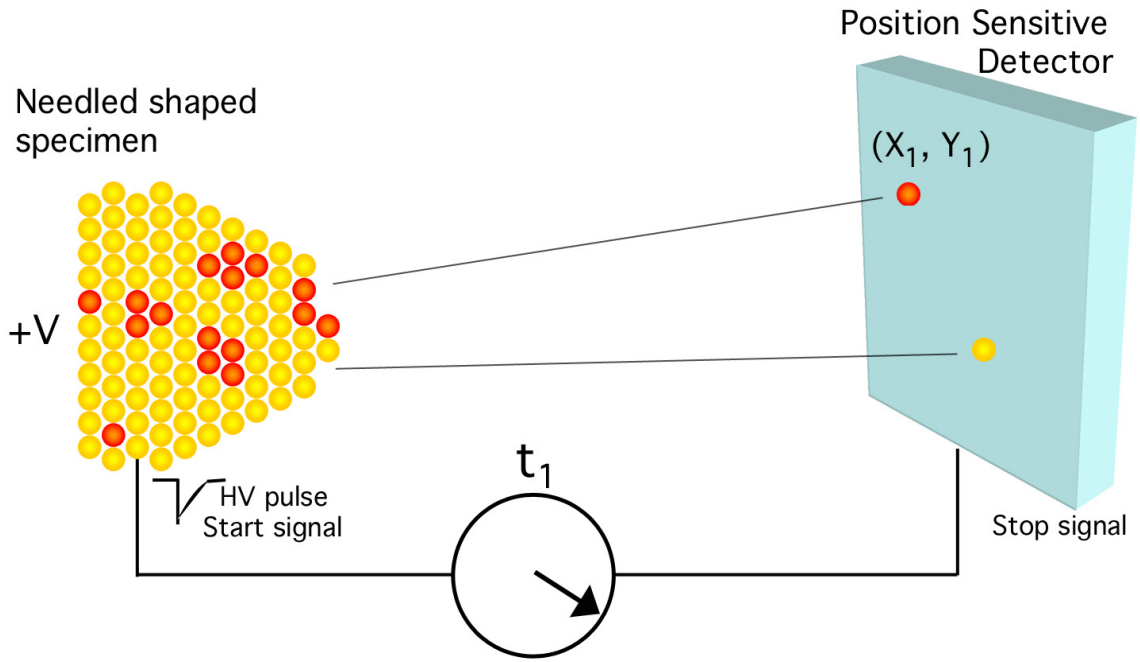
Atom Probe Tomography (APT)

- APT involves ionization of atoms from the surface of a sharp microtip
- Ions are repelled by the anode (tip) and drawn toward the cathode (electrode)



Time of flight → Chemical nature

Impact Position → Atom position on tip surface

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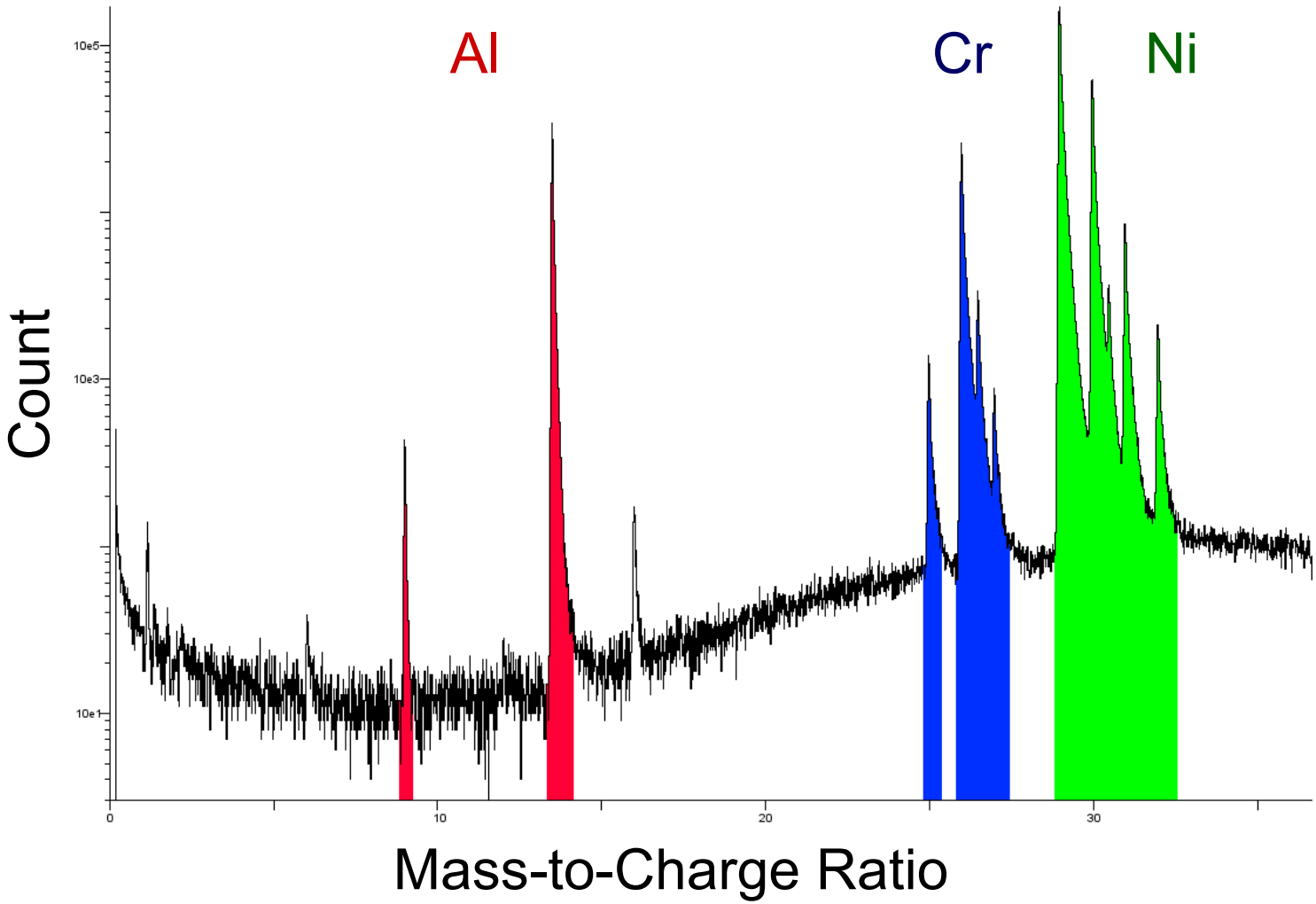
APT Mass Spectrum



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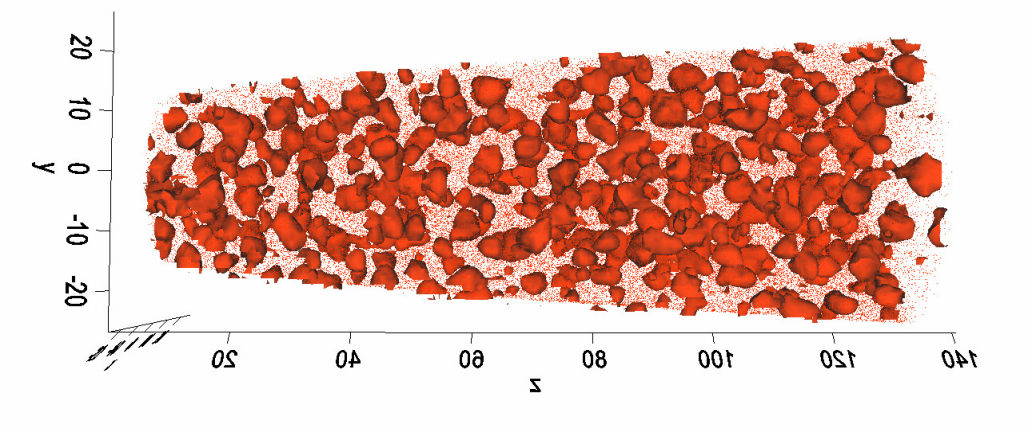
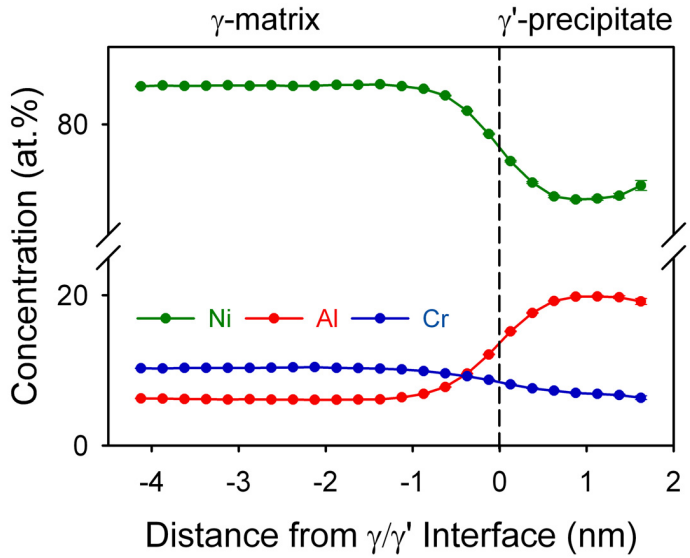
APT Results



APT micrograph of a model Ni-Al-Cr alloy aged at 600ºC for 4 h, with Ni and Cr atoms omitted for clarity, highlighting the γ'-precipitate phase with a 11.5 at.% aluminum isoconcentration surface.



The local composition across the γ/γ' interface.

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Atom Probe Tomography (APT)

- Phase transformation characterized over a range of aging times from 0 to 1024 hours by APT:

1) Nanostructure
   - precipitate morphology
   - average radius, $\langle R(t) \rangle$
   - precipitate number density, $N_v(t)$
   - precipitate volume fraction, ϕ

2) Composition
   - evolution of the γ and γ'-phases
   - equilibrium phase compositions
   - concentration profile at the γ/γ' interface

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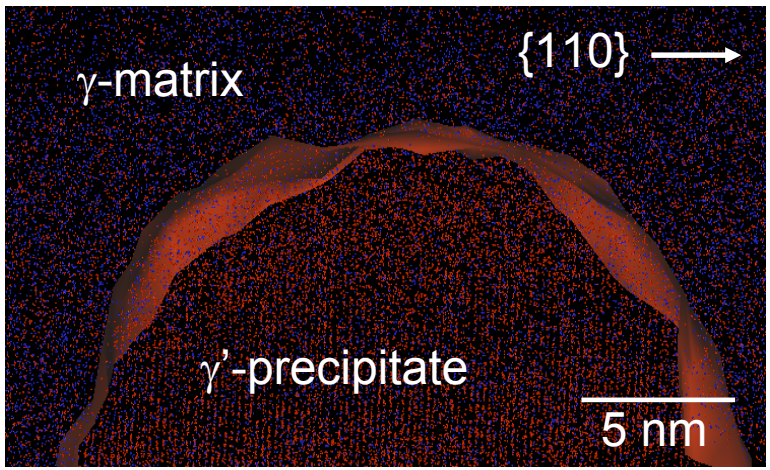
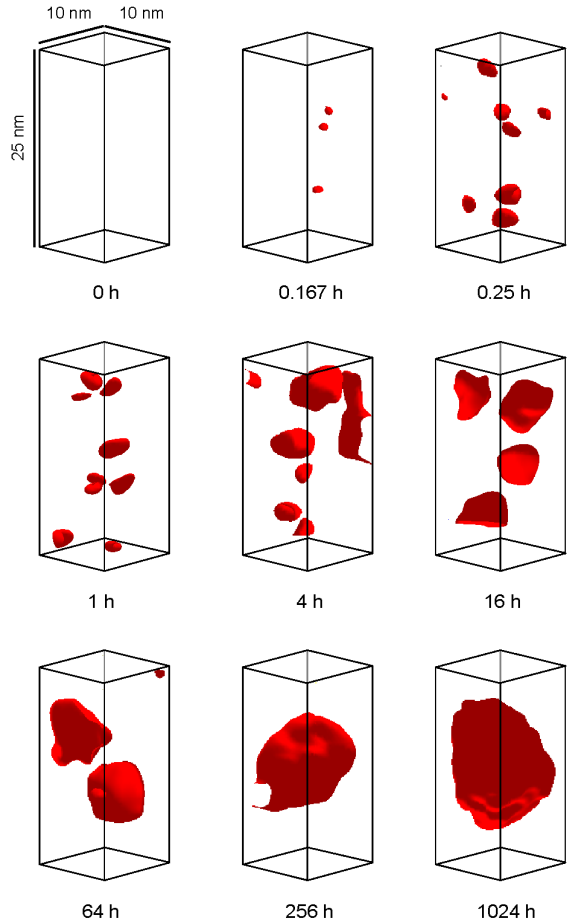
γ'-precipitate Morphology by APT

- Nanometer-sized spheroidal γ'-precipitates are detected in both alloys over the full range of aging times, from 1/6 to 1024 hours



A γ'-precipitate of radius ca. 9 nm is delineated by the dark 10.5 Al at.% isoconcentration surface, and shows {110} planes with an interplanar spacing of 0.26 nm.



The temporal evolution of the γ'-precipitate morphology in Ni-7.5 Al-8.5 Cr at.% aged at 600ºC.

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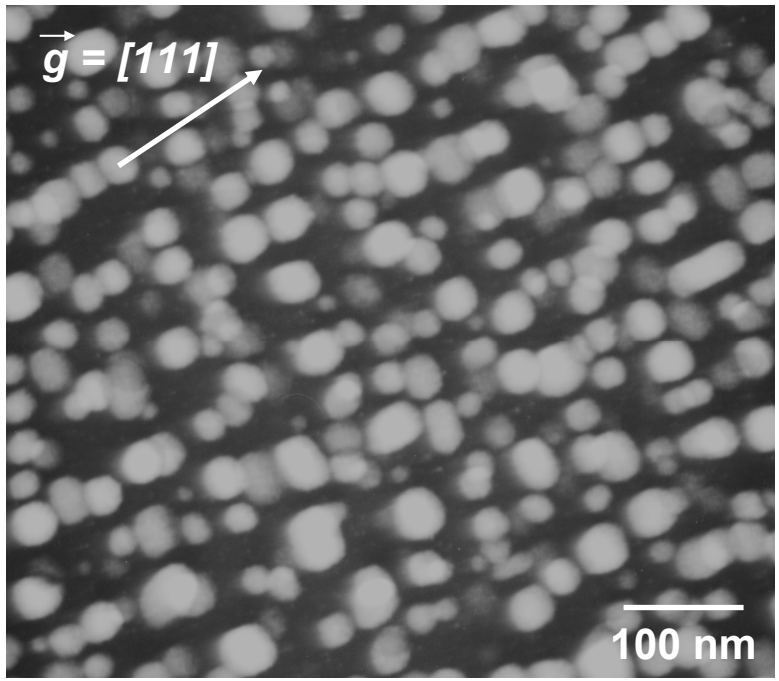
TEM

- TEM shows the spheroidal morphology of the γ'-precipitates is maintained to an aging time of 1024 h



A centered superlattice reflection dark–field image of spheroidal γ'-precipitates, for a Ni-7.5 Al- 8.5 Cr at.% sample aged for 1024 h at 600°C. Image recorded near the [011] zone axis, with **g** = [111] being the operating reflection.

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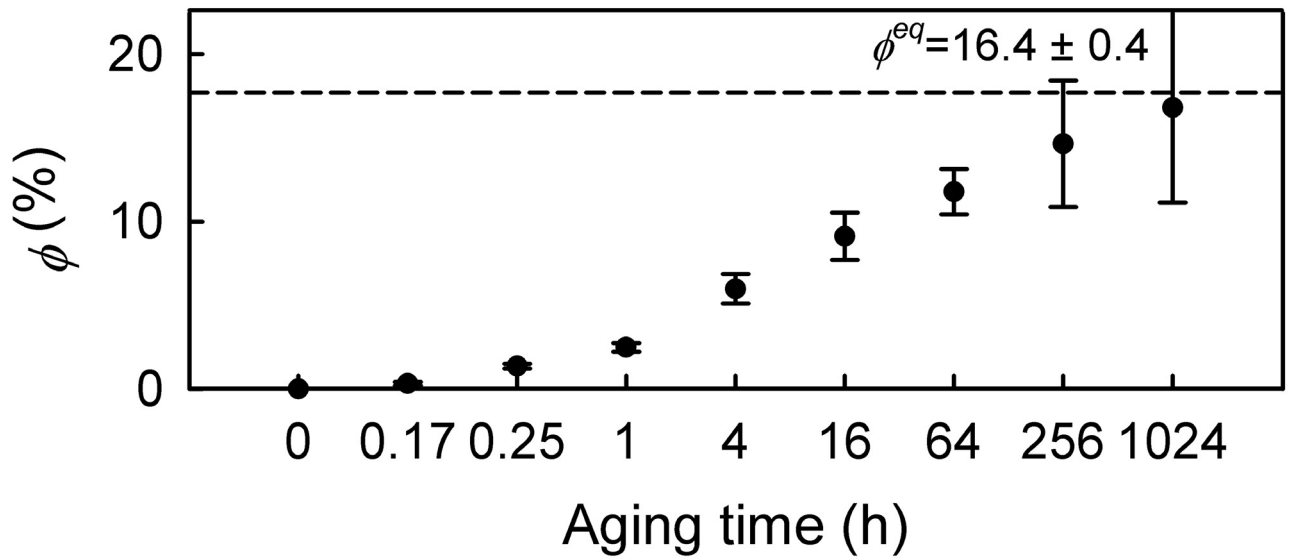
Precipitate Volume Fraction (ϕ)



- The value of ϕ continues to evolve with time, transformation not complete at an aging time of 1024 h

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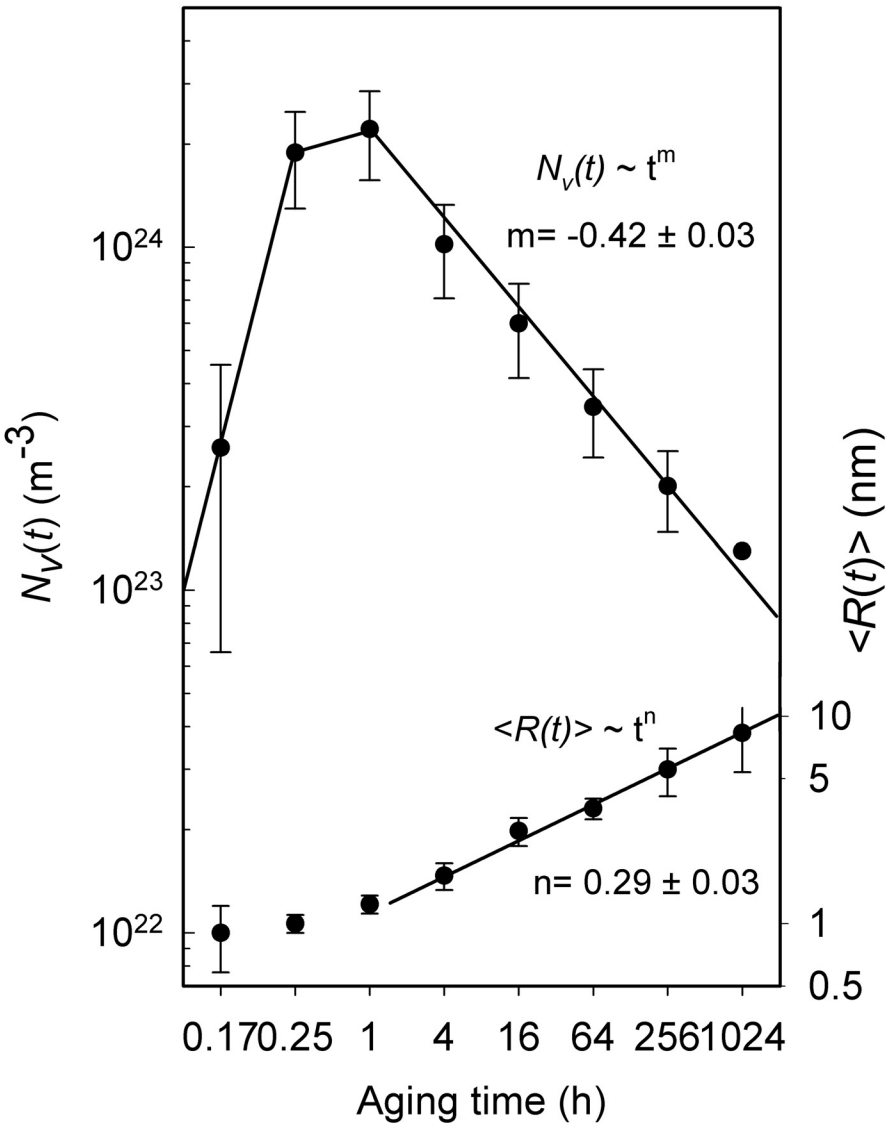
γ'-precipitate Number Density (N_v) and Radius <$R(t)$>



- A high maximum $N_v(t)$ of (2.2±0.6) x 10^{24} m^{-3} is achieved after aging for 1 h at 600°C
- Precipitate <$R(t)$> values range from 1-10 nm

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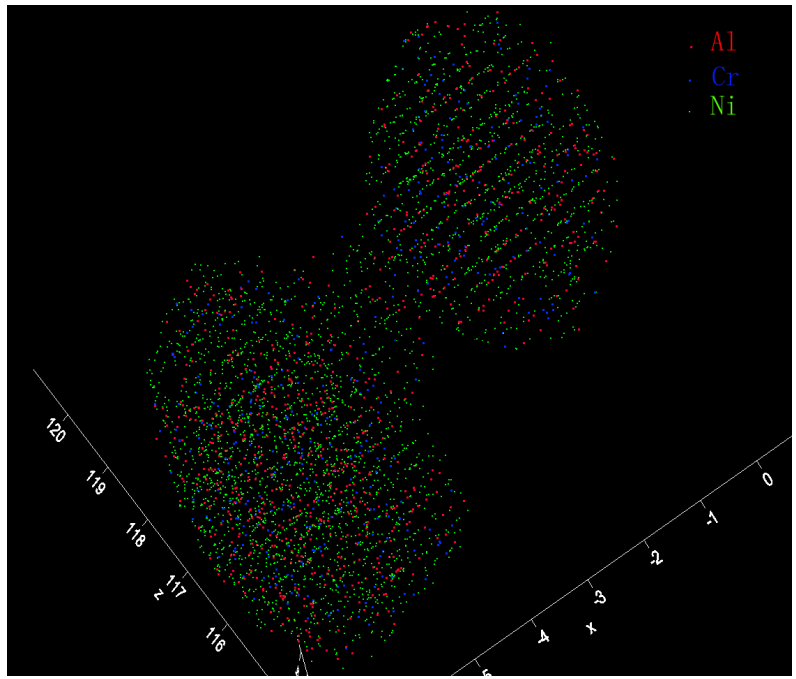
Precipitate Coalescence

- Precipitate coalescence at the outset of the coarsening regime in both alloys, characterized by the formation of “necked” regions which exhibit $L1_2$-type ordering.
- γ’-precipitate coagulation and coalescence is believed to result from the overlap of the diffusion fields associated with adjacent γ’-precipitates [5].



Atomic view of two γ’-precipitates coalescing together across a “neck” region in Ni-7.5 Al-8.5 Cr at.% after aging for 1 h at 600°

[5] Mao Z, Sudbrack C, Yoon K, Martin G, Seidman D. Diffusion Mechanism as a Selection Process for Nucleation, Growth and Coarsening Pathway in Multicomponent Concentrated Alloys. submitted to Nature Materials 2006.

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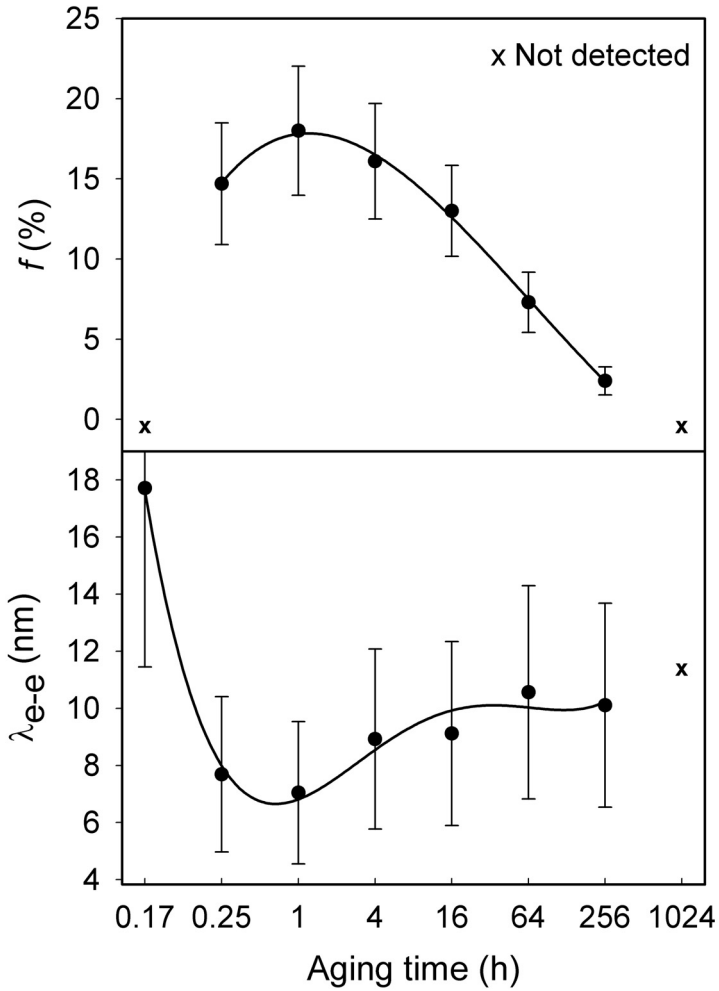
Precipitate Coalescence & Spacing

- The fraction of interconnected precipitates, *f*(%), achieves a maximum at 1 h, corresponding to minimum in the value of the interprecipitate spacing, $\lambda_{e\text{-}e}$, and the peak $N_v(t)$



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Calculated tracer D values: Ni-5.2 Al-14.2 Cr at.% @ 600°C

m^2/s	D_i
Ni	2.5×10^{-21}
Al	9.7×10^{-21}
Cr	3.0×10^{-21}

Thermodynamics : Ni-Data (N. Saunders)
Diffusion Mobilities: Ni-Mob database (NIST C. E. Campbell)

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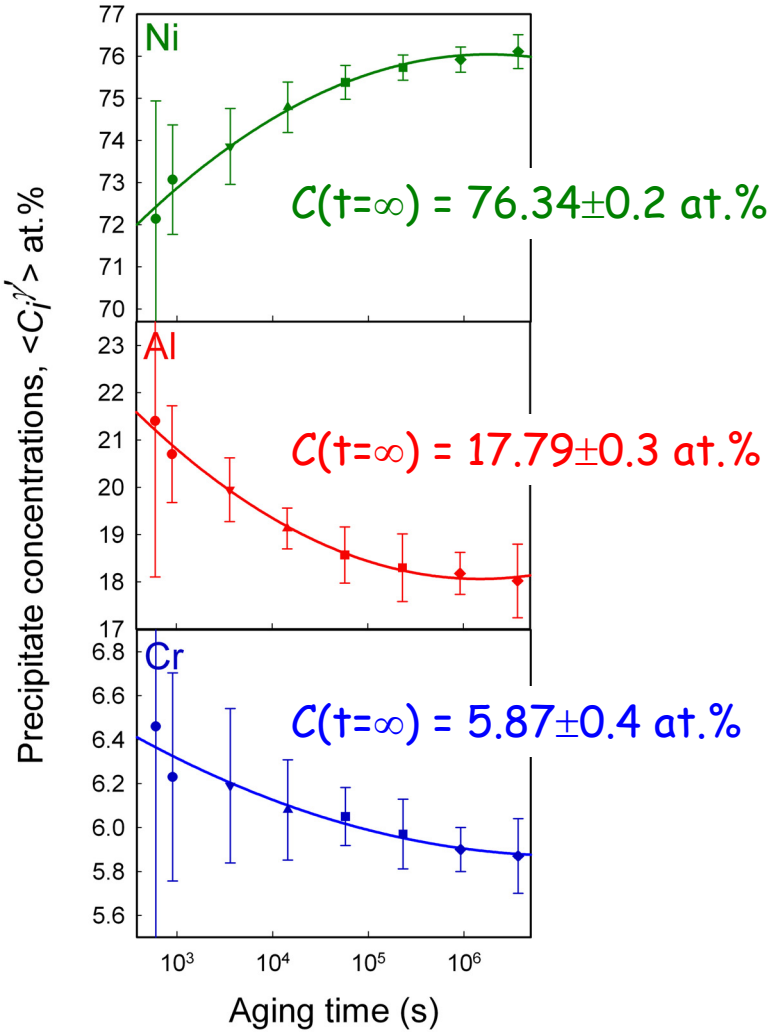
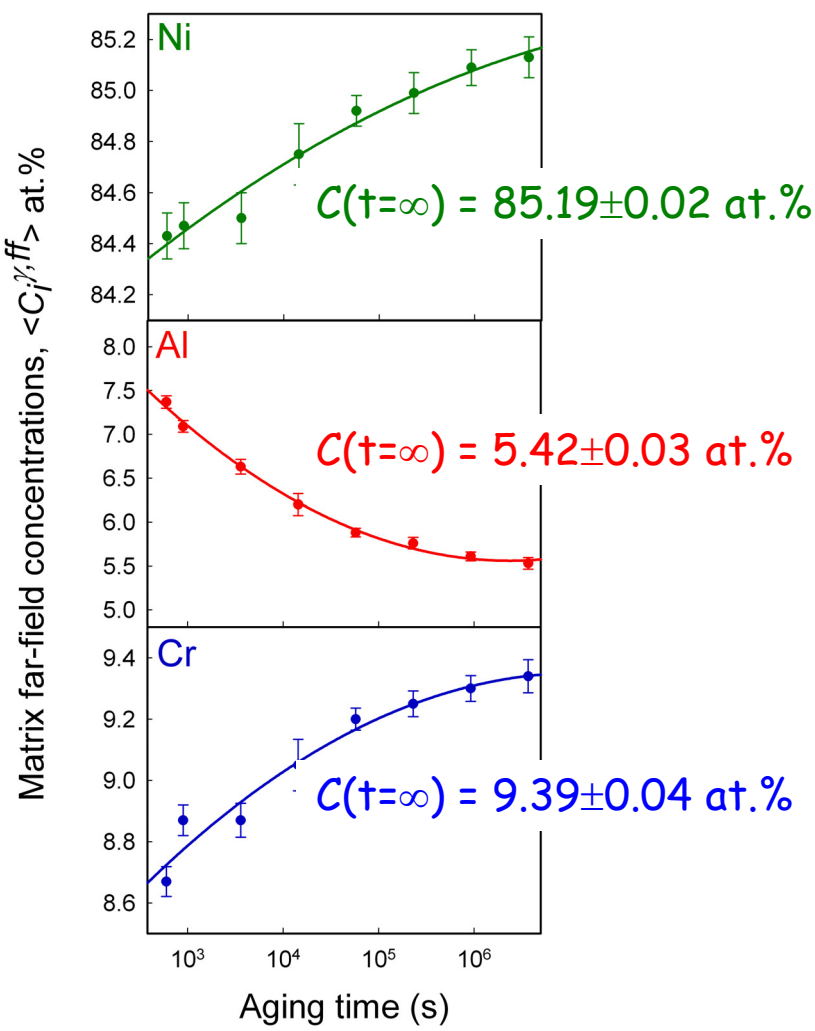
Compositional Evolution

γ'–precipitate



γ–matrix



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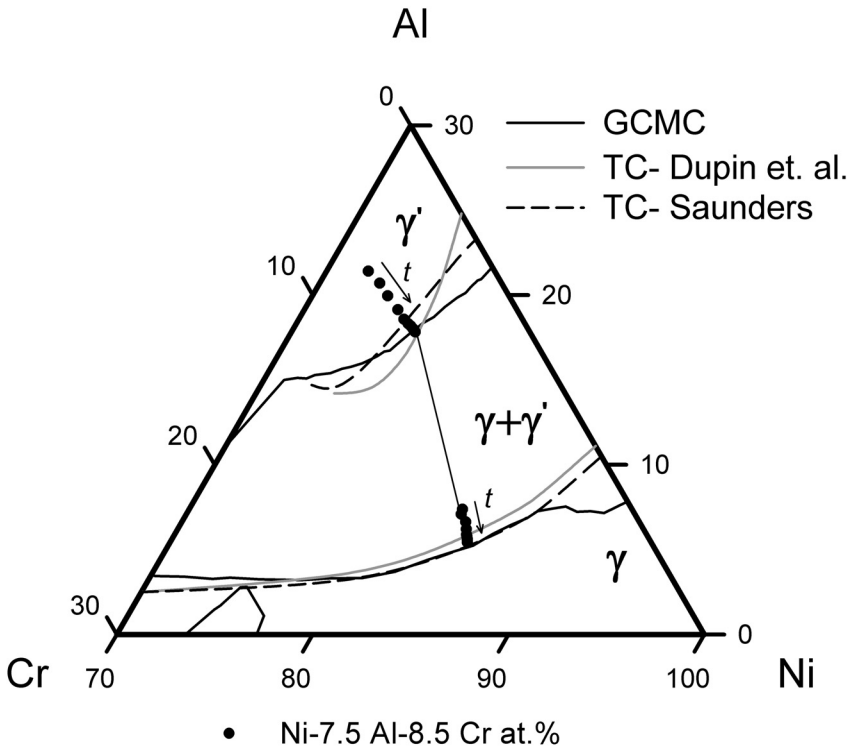
Compositional Phase Trajectory



The trajectories of the compositional evolution of the γ-matrix and γ'-precipitate phases of Ni-7.5 Al-8.5 Cr at.% on a partial Ni-Al-Cr ternary phase diagram at 600°C.

[4] Mao Z, Sinnott SB, Martin G, D.N. S. Determination of Pair-Wise Interaction Energies and the Calculation of Ternary Phase Diagrams of Ni-Al-Cr Alloys by First-Principles Calculations. to be submitted to Acta Materialia 2006.

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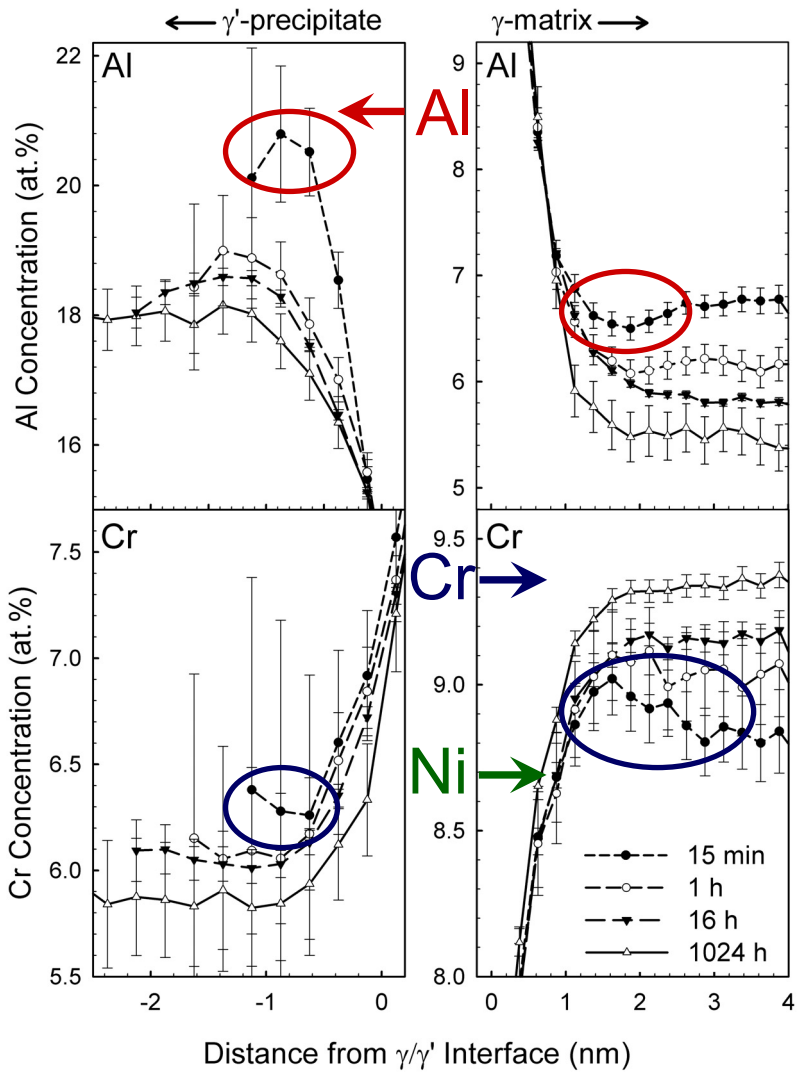
Interfaces in Ni-7.5 Al-8.5 Cr at.%

- γ-matrix and γ'-precipitate compositions continue to evolve with time
- A transient enrichment of chromium and a depletion of aluminum are observed on the γ-matrix side of γ/γ'-interfaces
- This transient behavior is believed to be a result of flux coupling



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Basic Conclusions from APT

- A spheroidal γ'-precipitate morphology is maintained over the full range of aging times, with some γ'-precipitate coalescence around the peak in number density
- APT allows for the quantification of the nanostructural and compositional evolution during phase decomposition

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Where does diffusion fit into this?

- In order to understand phase decomposition, it is essential to understand:

1) Thermodynamics (driving force for phase decomposition)
   - ThermoCalc
   - APT chemical characterization
2) Kinetics (nucleation and coarsening rates, coalescence)
   - Dictra
   - Comparison of APT experimental data and KMC data (Zugang)

Questions?